

# An Evaluation of CO<sub>2</sub> Sequestration in Organic-rich Shales Using COMSOL

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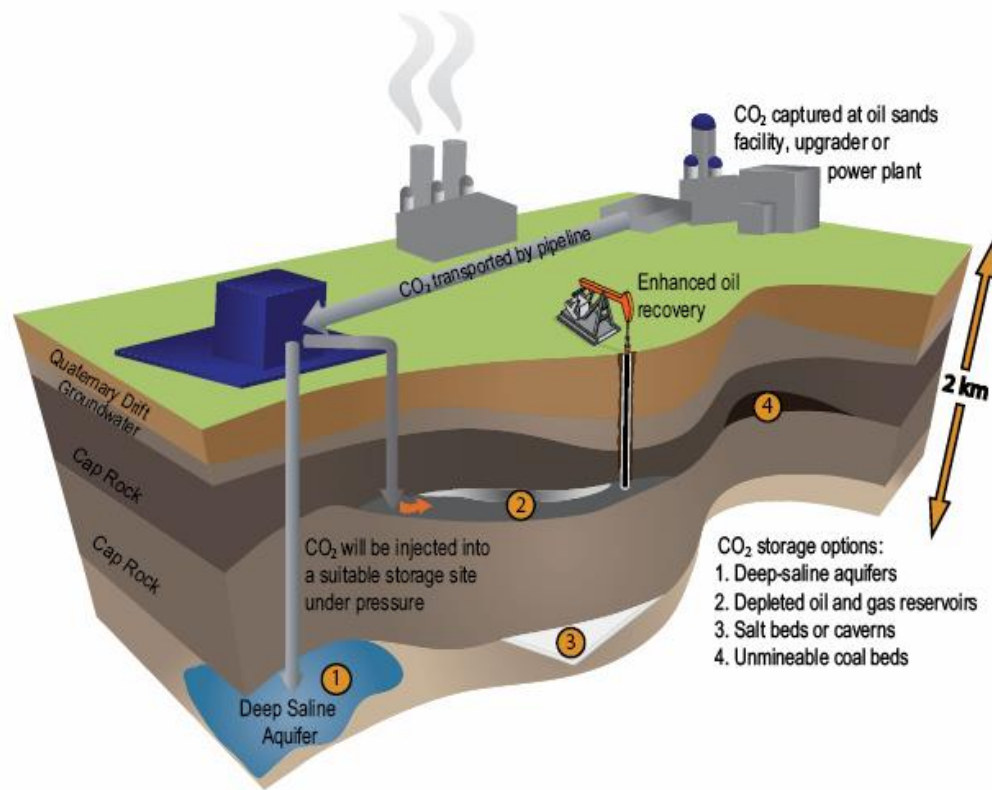
University of Kansas

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# Presentation Outline

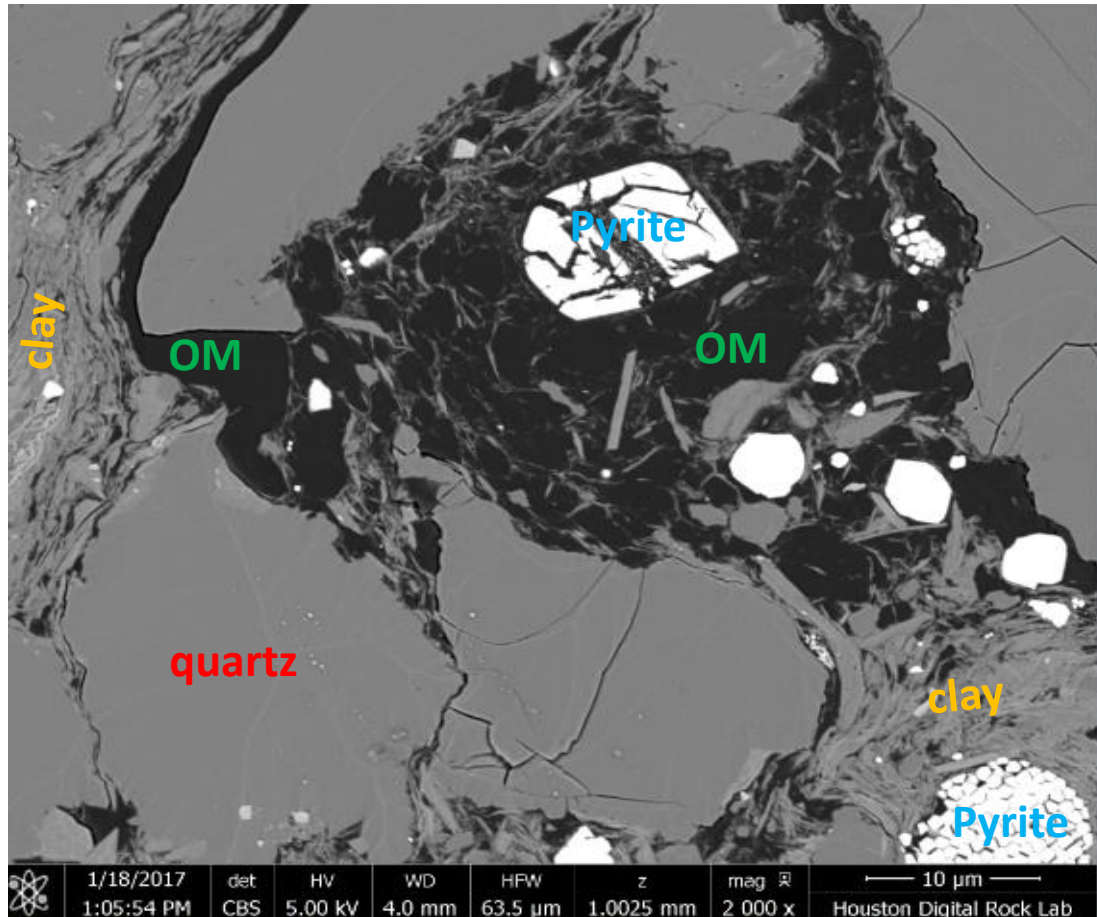
- Introduction
- Objective
- Method
- Results
- Discussion
- Summary

# Carbon dioxide (CO<sub>2</sub>) sequestration



- Involves separation and capture of CO<sub>2</sub> prior to atmospheric release
- Geologic storage include:
  - organic-rich shales
- Benefits of CO<sub>2</sub> sequestration:
  - Mitigate GHG emissions
  - Increased oil/gas recovery

# Organic-rich shales



BSE image of a Chattanooga shale sample

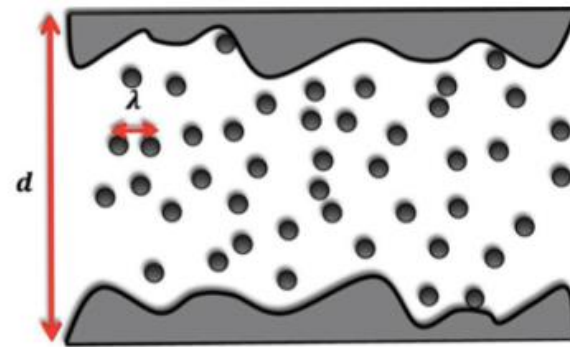
- Consist of organic matter (OM) and mineral matrix
- Organic matter (OM) produces hydrocarbons (oil & gas)
- Degenerated organic matter leaves behind nano-pores
- OM preferentially adsorbs  $\text{CO}_2$  over methane ( $\text{CH}_4$ )
- Ultra-tight nature minimizes leakage



# Objective

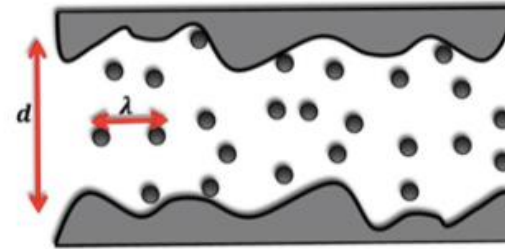
- To understand the underlying mechanism(s) of CO<sub>2</sub> sequestration in organic-rich shales at varying pressure and temperature using COMSOL

# Flow regimes



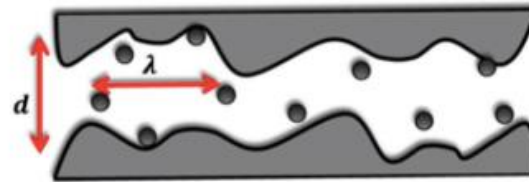
$$K_n \leq 0.01$$

(a)



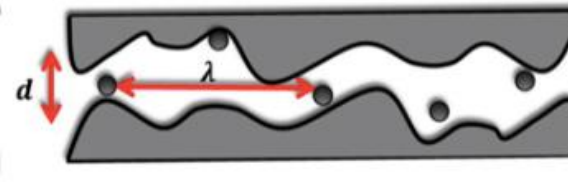
$$0.01 \leq K_n \leq 0.1$$

(b)



$$0.1 \leq K_n \leq 10$$

(c)



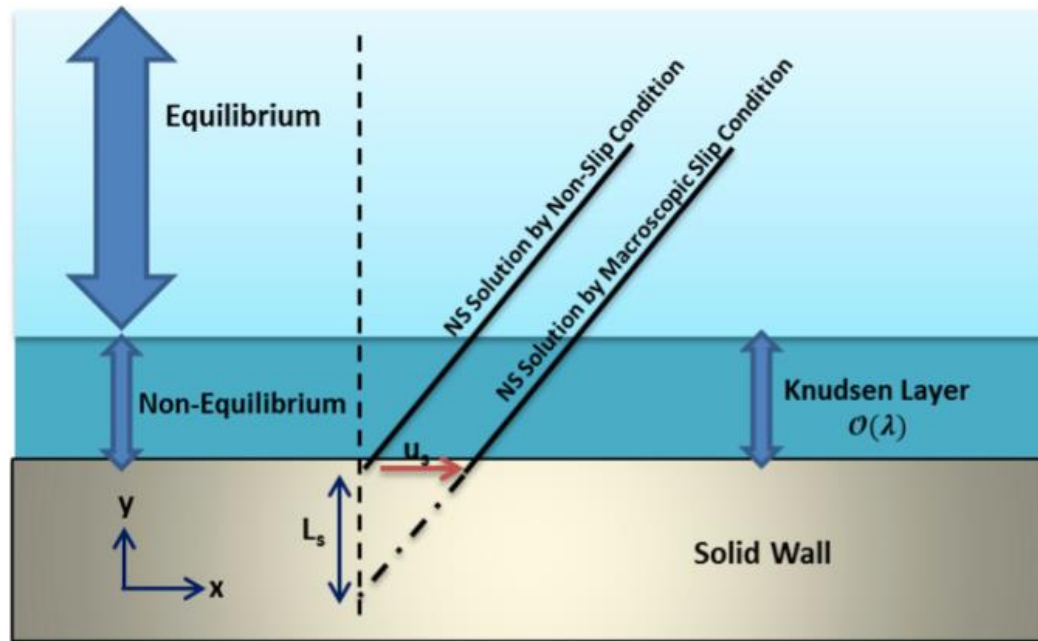
$$10 \leq K_n$$

(d)

- (a) Continuum flow
- (b) Slip flow
- (c) Transition flow
- (d) Free molecular flow

Schematic diagram of flow regimes  
(Moghaddam & Jamiolahmady, 2016)

# Knudsen layer



Schematic diagram of Knudsen layer  
(Moghaddam & Jamiolahmady, 2016)

- Non-equilibrium region, where wall collision is considered
- Covers less than 20% of characteristic length in slip flow
- Slip effects are more pronounced as Knudsen number increases

# Slip flow module - COMSOL

- Navier-Stokes applies but slip boundary condition is required.
- Maxwell first order slip boundary condition

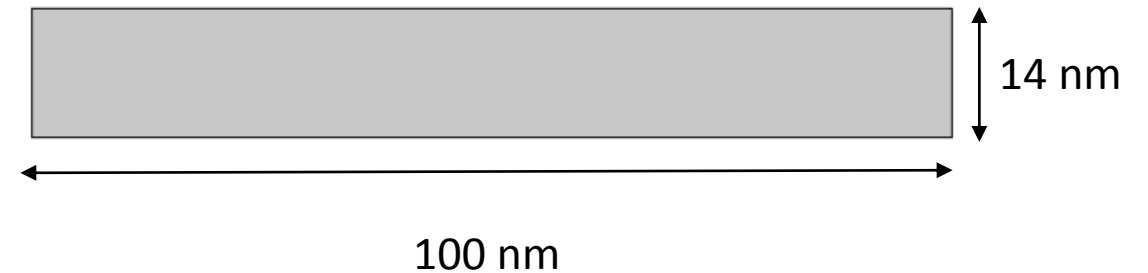
- $$U_{slip} = \frac{2-\sigma_v}{\sigma_v} \lambda \frac{\partial U}{\partial y}$$
- $$U_{slip} = U_{fluid} - U_{wall}$$

where,  $\sigma_v$  = tangential momentum accommodation coefficient



# Simulation

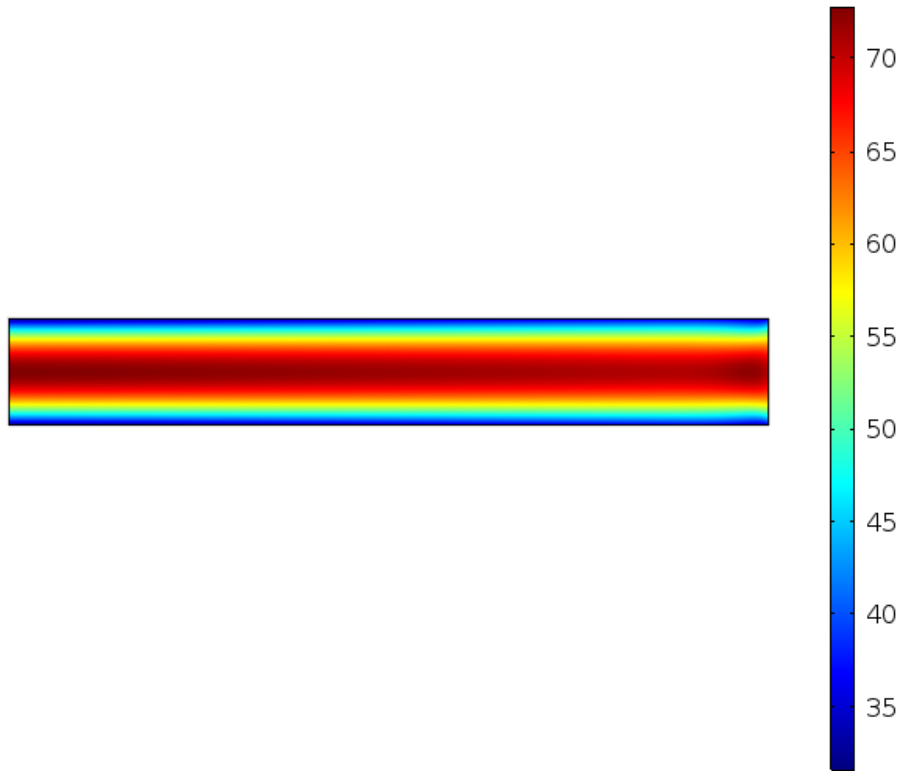
- Fluid domain within the pore-slit driven by pressure gradient
- Fluid domain : CO<sub>2</sub> and CH<sub>4</sub> gases
- Pressures vary from 250psi to 500psi
- Temperature vary from 298K to 320K
- TMAC varied from 0.9 to 0.7



Model geometry

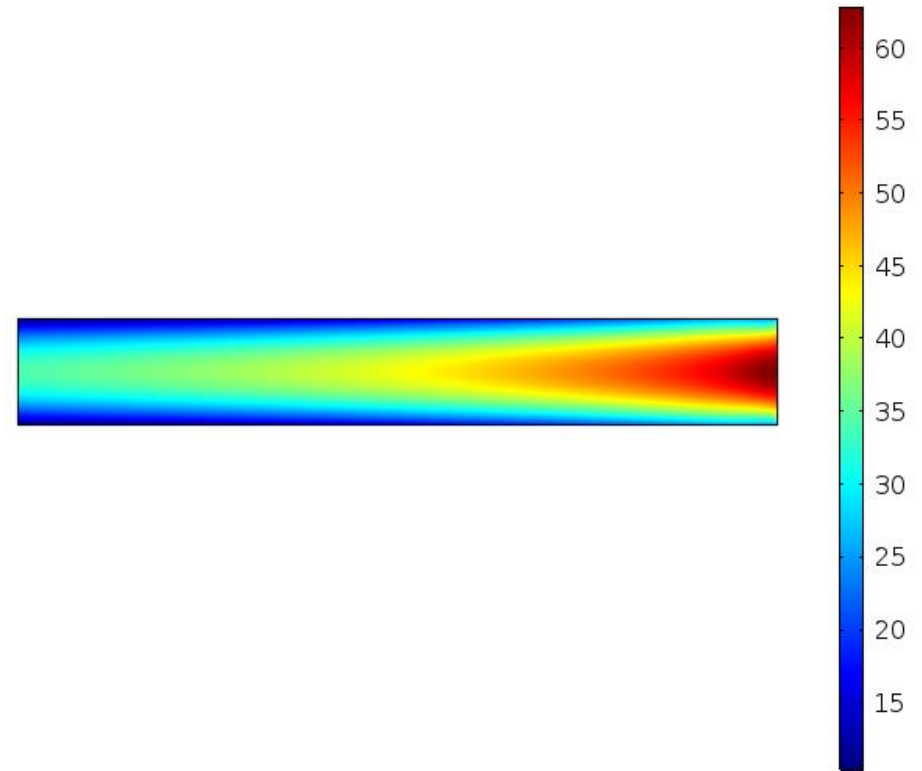
# Results

Surface: Velocity magnitude (m/s)



Velocity magnitude of CH<sub>4</sub> at 250 psi, 298.15 K, and TMAC = 0.9

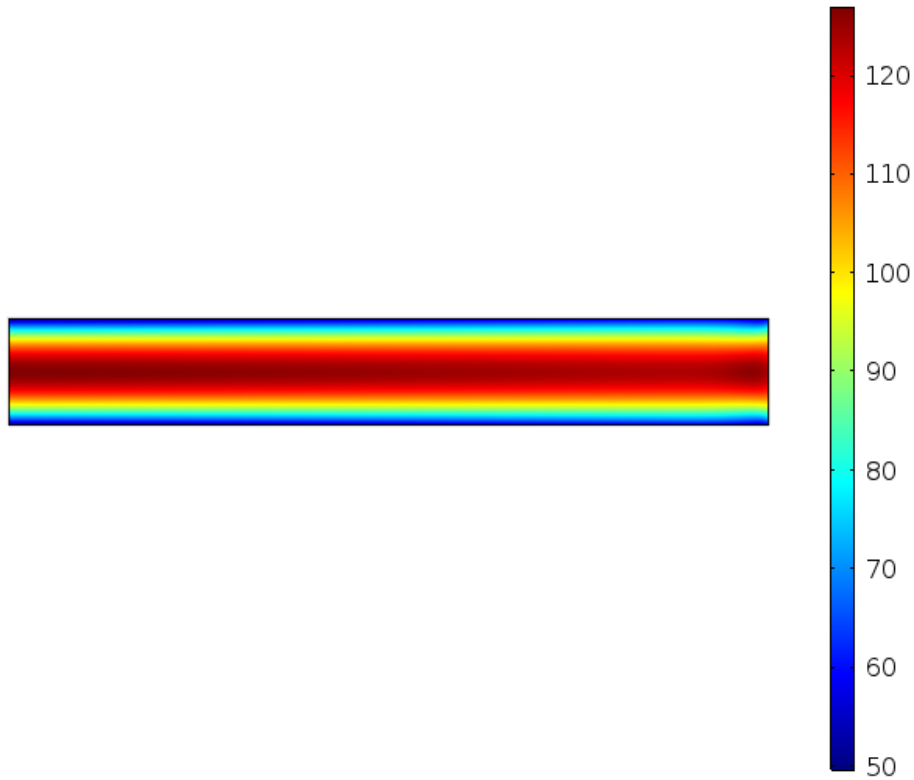
Surface: Velocity magnitude (m/s)



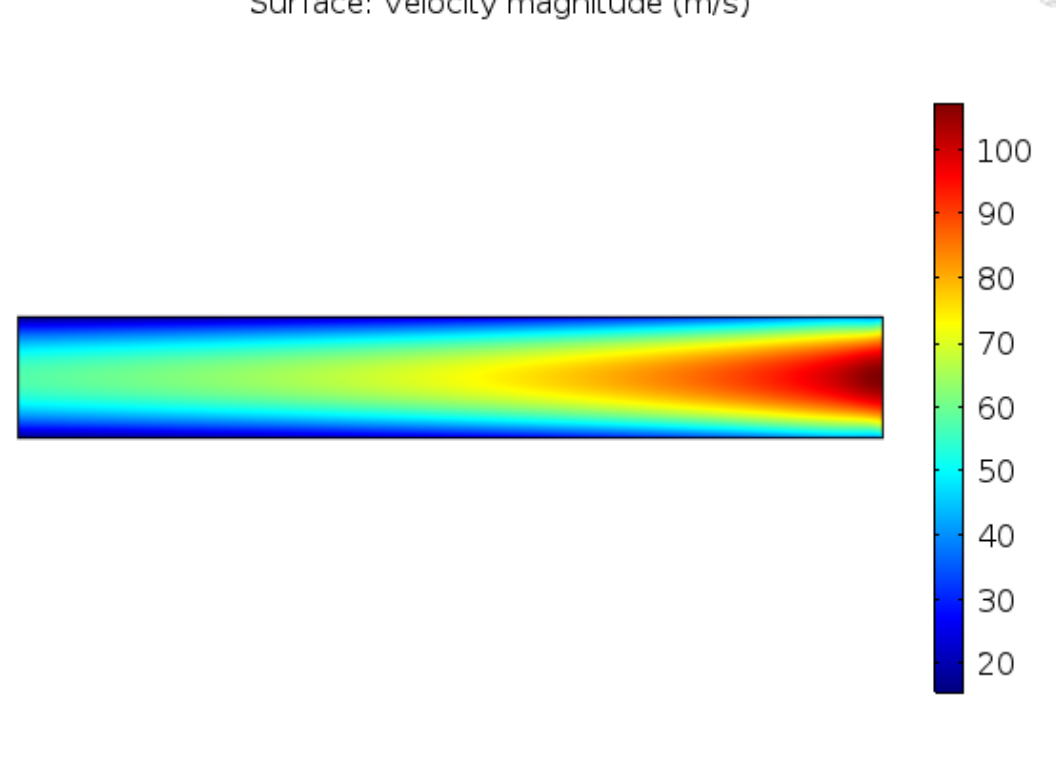
Velocity magnitude of CO<sub>2</sub> at 250 psi, 298.15 K and TMAC = 0.9

# Results

Surface: Velocity magnitude (m/s)

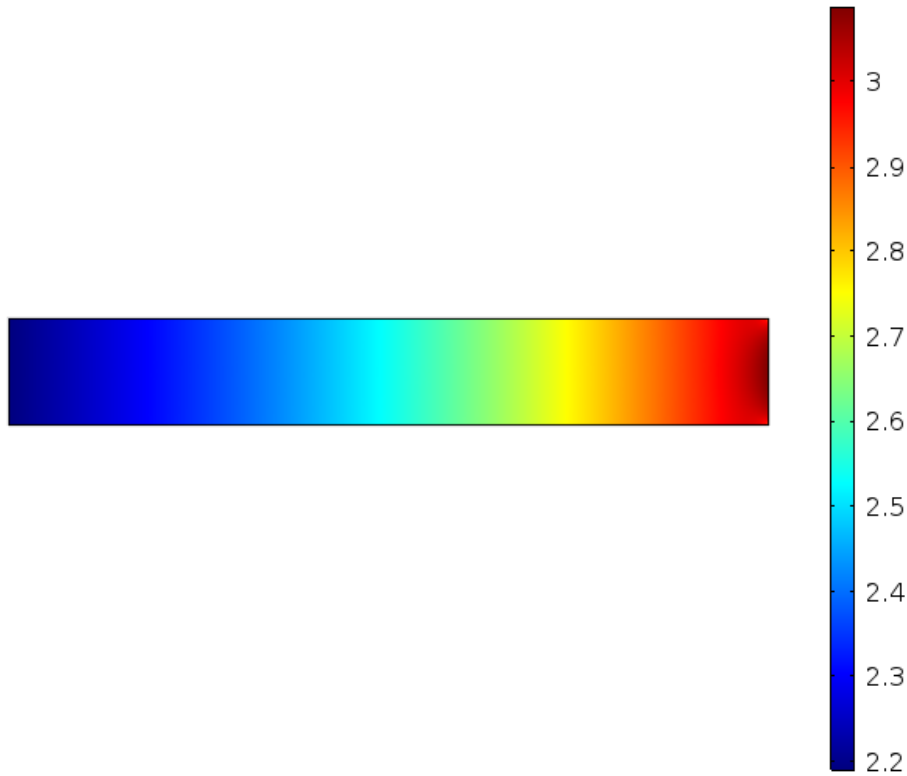


Surface: Velocity magnitude (m/s)



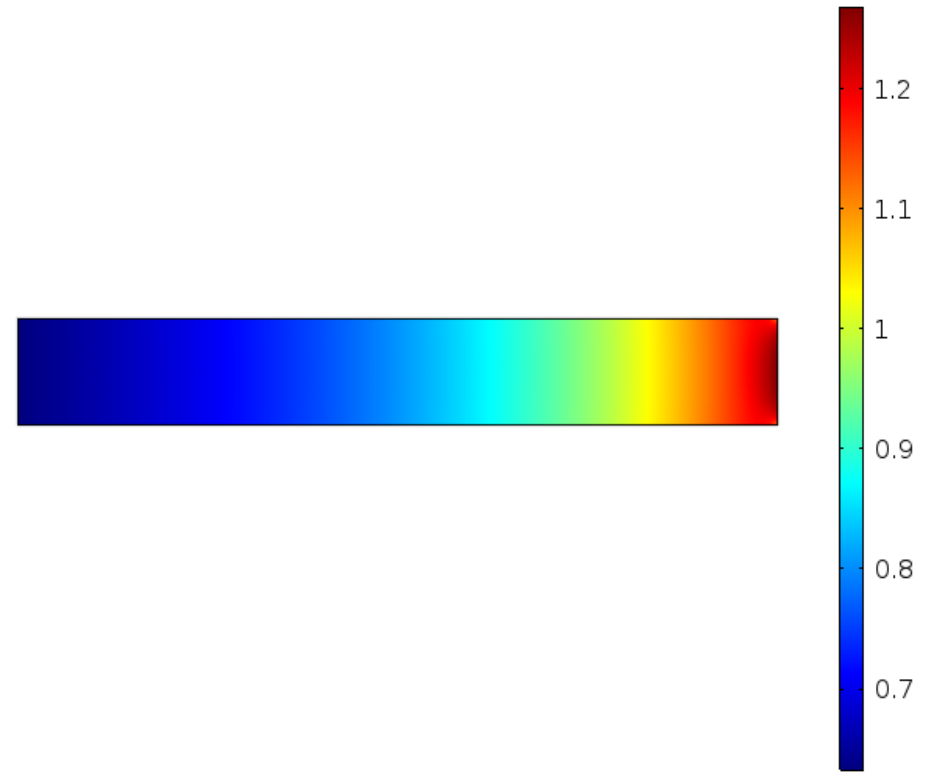
# Results

Surface: Mean free path (nm)



Mean free path of CH<sub>4</sub> at P=500 psi, T=298.15K, and TMAC=0.9

Surface: Mean free path (nm)



Mean free path of CO<sub>2</sub> at P=500 psi, T=298.15K, and TMAC=0.9

# Discussion

- At the same prevailing conditions, CH<sub>4</sub> recorded higher slip velocity and mean free path than CO<sub>2</sub>
- Decrease in TMAC from 0.9 to 0.7 slightly caused an increase in slip velocity and mean free path in both cases
- Increase in temperature from 298.15 K to 320 K also saw an increase in the slip velocity and mean free path in both cases
- Increase in pressure from 250 psi to 500 psi resulted in a decrease in the mean free path
- Knudsen number ranged from 0.06 to 0.1

# Summary

- Carbon dioxide ( $\text{CO}_2$ ) is more susceptible to adsorption than methane ( $\text{CH}_4$ ) in the same pore geometry and under similar conditions.
- TMAC plays an important role in gas slip models
- Slip velocity is due to pore wall interactions and therefore depends on the type of reflection gas molecules experience at the walls

# Acknowledgements





**THANK YOU FOR YOUR  
ATTENTION.**

**QUESTIONS ??**